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TRANSIENT UNSATURATED COUPLED HEAT AND MOISTURE FLOW - MODEL CALIBRATION

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ABSTRACT

The results of the granite block experiment conducted by Carleton University was used to validate the computer code TRUCHAM developed at Ontario Hydro. The thermohydraulic material properties of the reference buffer mix used in the experiment were determined by McGill University, Carleton University and Ontario Hydro. Good agreement was obtained between the measured and the predicted temperature regime within the granite block, and the moisture regimes within the buffer. The results of this study provide further confidence on the validity of the computer code TRUCHAM and the thermohydraulic material properties of the reference buffer mix determined by Ontario Hydro.

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TRANSIENT UNSATURATED COUPLED HEAT AND MOISTURE FLOW - MODEL CALIBRATION

1.0 INTRODUCTION

In the proposed borehole emplacement scheme (TEC-2) of the Canadian nuclear fuel waste disposal vault concept, the thermal performance of the buffer barrier will have a significant effect on the vault design. To assess the thermal performance of the emplacement scheme, full scale buffer/container experiments will be conducted at the Underground Research Laboratory, URL/1/. An analytical computer model, TRUCHAM, developed by Ontario Hydro Research Division will be employed to predict the thermal performance of the experiments/2/.

The thermal conductivity of a soil is a function of its moisture content/3,4/. Under temperature gradients, the moisture in a soil medium tends to redistribute which in turn alters the thermal properties and the thermal regime. Thus a coupled heat and moisture transport process is set up in the partially saturated soil/5,6,7/. Thermally induced soil water movement in partially saturated soil is a complex phenomenon. Based on Fick's law, Philip and deVries proposed a set of governing equations to describe the phenomenon of heat and moisture flow through porous medium/8/. These equations are:

$$\partial\theta/\partial t = \nabla.(D_T \nabla T) + \nabla.(D_\theta \nabla\theta) + \partial k/\partial z \quad (1)$$

$$c\,\partial T/\partial t = \nabla.(\lambda \nabla T) - L\,\nabla.(D_{\theta\,vap}\,\nabla\theta) \quad (2)$$

where ∇T = thermal gradient

$\nabla\theta$ = volumetric moisture content gradient

θ = volumetric moisture content

T = temperature

k = hydraulic conductivity

c = volumetric heat capacity

λ = thermal conductivity

$D_T = D_{Tliq} + D_{Tvap}$

D_{Tliq} = thermal liquid diffusivity

D_{Tvap} = thermal vapour diffusivity

$D_\theta = D_{\theta\,liq} + D_{\theta\,vap}$

$D_{\theta\,liq}$ = isothermal liquid diffusivity

$D_{\theta\,vap}$ = isothermal vapour diffusivity

Equations 1 and 2 describe the heat and moisture transfer in partially saturated soils. In view of the coupling effect between Equations 1 and 2 and the non-linear material properties involved, no close form solution can be obtained for most practical situations. Alternatively, numerical techniques are employed to solve this set of equations.

A computer code, TRUCHAM was developed at Ontario Hydro/2/ which utilizes an integrated finite difference technique. The special features of this program are: (1) it can successfully deal with coupled heat and moisture induced flow; (ii) it can accommodate a wide variation of material properties; (iii) its formulation in multi-dimensions is relatively simple, and (iv) there is an automatic choice of time step to ensure the stability and convergence of the numerical solution/2/.

The thermohydraulic material properties of the reference buffer mix are required to use the computer code to predict the thermal performance of the buffer. One-dimensional diffusion experiments were conducted at McGill University, Carleton University and Ontario Hydro/9,10,11/. These experiments were conducted on specimens of reference buffer material (50% sand and 50% Avonlea bentonite) compacted to a reference dry density of 1680 kg/m^3 at 18.3% moisture content. The results of these experiments are summarized in Figures 1 and 2. The thermal conductivity versus volumetric moisture content relationship of the reference buffer material was determined by Ontario Hydro (Figure 3).

A number of large scale laboratory model experiments have been performed at Ontario Hydro and Carleton University to study the thermal performance of the reference buffer under simulated conditions/12,13/. Carleton University recently performed a single heater experiment in a granite block in which both the temperature and moisture were measured. In this study, the computer code TRUCHAM is used along with the thermohydraulic material properties determined by the various research groups to model the granite block experiment/13/. The objectives of this study are: (1) to assess the thermohydraulic material properties, and (2) to evaluate the validity of the computer code,

2.0 THE GRANITE BLOCK EXPERIMENT

In 1989, Carleton University conducted a granite block experiment to assess the thermal performance of the reference buffer in the borehole emplacement scheme of the TEC-2 design. The layout of the experiment is shown in Figure 4. The granite block had the cross sectional dimensions of 918 mm x 926 mm and a height of 2446 mm. It contained a central borehole 262 mm in diameter and 975 mm in depth. A cylindrical electric heater was placed in the borehole providing a heat source to simulate the heat generated by a nuclear fuel waste container. The annular space between the heater and the borehole wall was filled with reference buffer material (50/50 Avonlea bentonite and silica sand) compacted to the reference dry density and moisture content of 1680 kg/m^3 and 18.3% respectively. The temperature regime within the granite block and the heater was monitored by an array of thermocouples. No thermocouple was placed in the buffer. At completion of the experiment, moisture regime within the buffer was determined by performing moisture content tests on core samples obtained at different locations within the buffer. The experiment was conducted with a constant heater temperature of 100 °C and lasted for about 2200 hours.

3.0 COUPLED ANALYSIS WITH AVERAGE THERMOHYDRAULIC MATERIAL PROPERTIES

3.1 PERMEABLE HYDRAULIC BOUNDARY

In this section, the thermohydraulic material properties of the reference buffer mix determined by McGill University, Carleton University and Ontario Hydro are assessed. To simplify the study, three analyses were performed by using the average thermohydraulic material properties determined by each of the three research laboratories. The average thermohydraulic properties used in these analyses are defined as those measured at 40°C with an initial volumetric moisture content of 0.2. These average thermohydraulic material property values are:

Thermohydraulic Diffusivity	McGill University	Carleton University	Ontario Hydro
D_θ/L_{ww} (cm^2/sec)	$1x10^{-7}$	$1x10^{-8}$	$1.5x10^{-7}$
D_T/L_{wT} ($cm^2/sec/K$)	$1x10^{-5}$	$9x10^{-6}$	$1x10^{-5}$

The hydraulic boundary condition at the buffer/rock interface was assumed to be permeable (as was found from the results of the experiments) and the buffer was assumed to be saturated at a volumetric moisture content of 0.4.

A constant thermal conductivity value of 3.5 w/m/°C was assumed for the granite. A set of thermohydraulic material properties was assumed for the granite such that a permeable hydraulic boundary condition is created at the buffer/rock interface. The element mesh used in this study is shown in Figure 5.

3.2 Results

The measured and predicted temperatures versus time relationship at various locations in the granite block are plotted in Figures 6, 7, 8 and 9.

The predicted temperatures versus time relationship based on the average thermohydraulic properties from McGill University and Ontario Hydro show a pronounced peak at elapsed time of 1100 hours and 500 hours respectively (Figures 8 and 9). The predictions based on the average thermohydraulic properties determined by Carleton University shows no peak in the temperature versus time curves (Figure 7). The measured and predicted temperatures at location 1 in the granite block (Figure 6) are summarized below:

	Peak temperature at location 1 in rock (Figure 6)	time of occurrence	temperature at 2200 hours
Measured	72 °C	500 hours	64 °C
Predicted			
Carleton**	----------	no peak ----------	
McGill**	71 °C	1100 hours	68 °C
Hydro**	69 °C	500 hours	62 °C

**using average thermohydraulic properties

The normalized volumetric moisture content profiles of the 3 analyses (at time = 2200 hours), plotted in Figures 10, 11 and 12, clearly indicate moisture migration in the buffer. By comparing these predicted moisture profiles to those measured (Figure 13), it can be concluded that the predictions based on Carleton University's data underestimate the amount of moisture loss in the buffer. The predictions based on average thermohydraulic properties from McGill University and Ontario Hydro, over estimate the amount of moisture loss in the buffer around the heater and under estimate the amount of moisture loss in the buffer above and below the heater.

3.3 Impermeable Hydraulic Boundary

In order to determine the effect of hydraulic boundary condition at the buffer/rock interface on the thermal regime in buffer, an analysis was made with the average thermohydraulic material properties determined by Ontario Hydro, and with an impermeable hydraulic boundary condition at the buffer/rock interface. The resulting temperature versus time curves are shown in Figure 14. The normalized volumetric moisture content regime at 2200 hours is plotted in Figure 15 which shows no sign of

thermal drying of the buffer. These results support the assumption of a permeable hydraulic boundary condition at the buffer/rock interface in the Carleton's experiment.

4.0 COUPLED ANALYSIS WITH THERMOHYDRAULIC MATERIAL PROPERTIES FROM ONTARIO HYDRO

A fully coupled heat and moisture analysis was performed with the thermohydraulic material properties determined by Ontario Hydro. The hydraulic boundary condition at the buffer/rock interface was considered to be permeable and the saturated volumetric moisture content of the buffer was assumed to be 0.4. The resulting temperature versus time curves for thermocouple locations 1 to 4 in the granite block (Figure 6) are plotted in Figure 16, and the normalized volumetric moisture content profile is shown in Figure 17. These figures show good agreement between the predicted and measured temperature and moisture regimes.

5.0 CONCLUSIONS

In this study, the results from the granite block experiment performed at Carleton University was used to evaluate the TRUCHAM code, and the thermohydraulic materic' properties determined by McGill University, Carleton University, and Ontario Hydro. Based on the results of this study the following conclusions are drawn:

(1) The temperature regime in the granite block and moisture regime in the buffer barrier can be predicted, within a reasonable range, by using the average thermohydraulic material properties determined by Ontario Hydro and McGill University.

(2) The hydraulic boundary condition at the buffer/rock interface has a significant influence on the occurrence of thermal drying of the buffer.

(3) The computer code TRUCHAM with the thermohydraulic material properties determined by Ontario Hydro can adequately model the coupled heat and moisture transport process in the buffer. The predictions match closely the thermal drying of the buffer observed in this large scale experiment.

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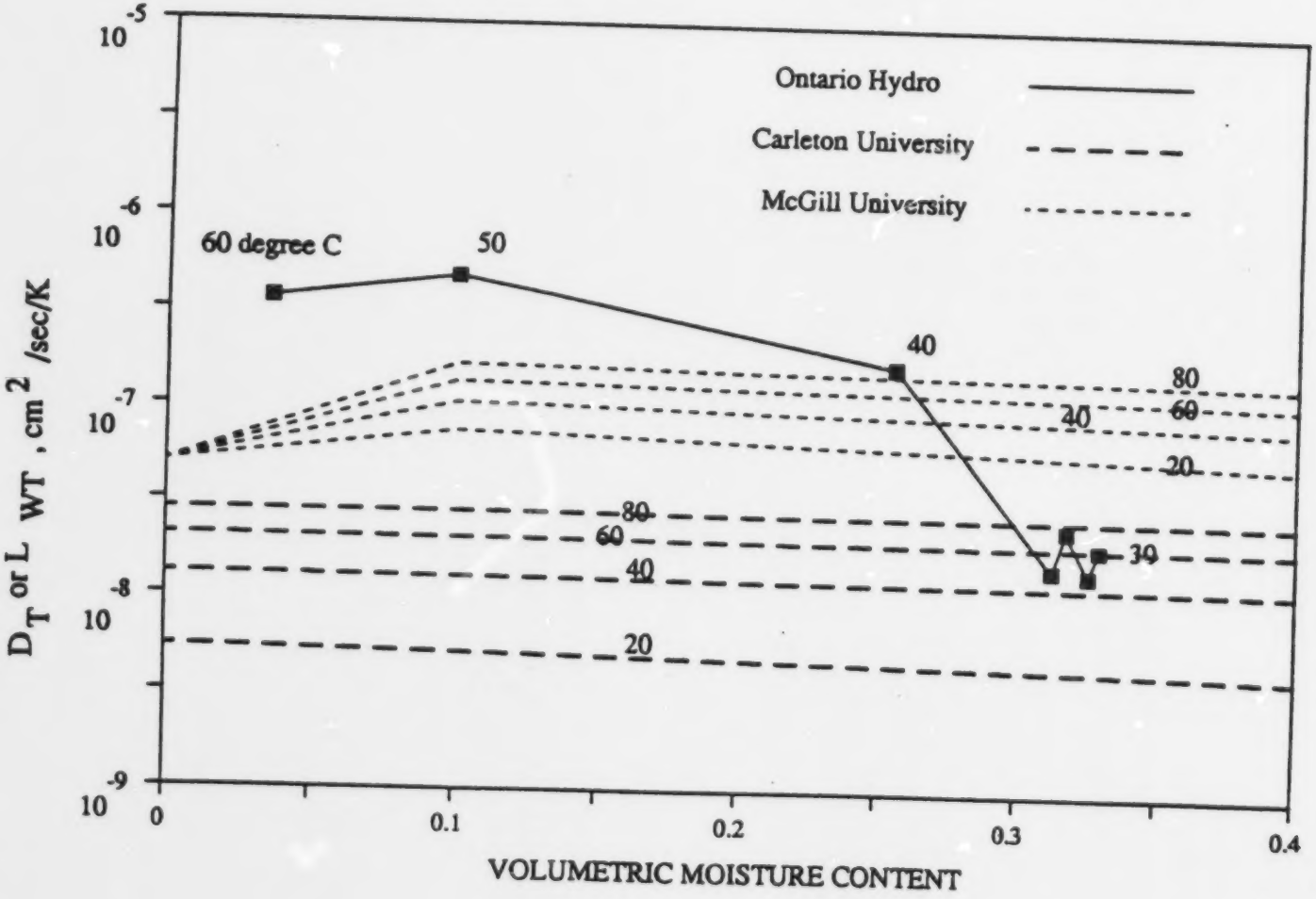

Figure 1 The D_T or L_{WT} values.

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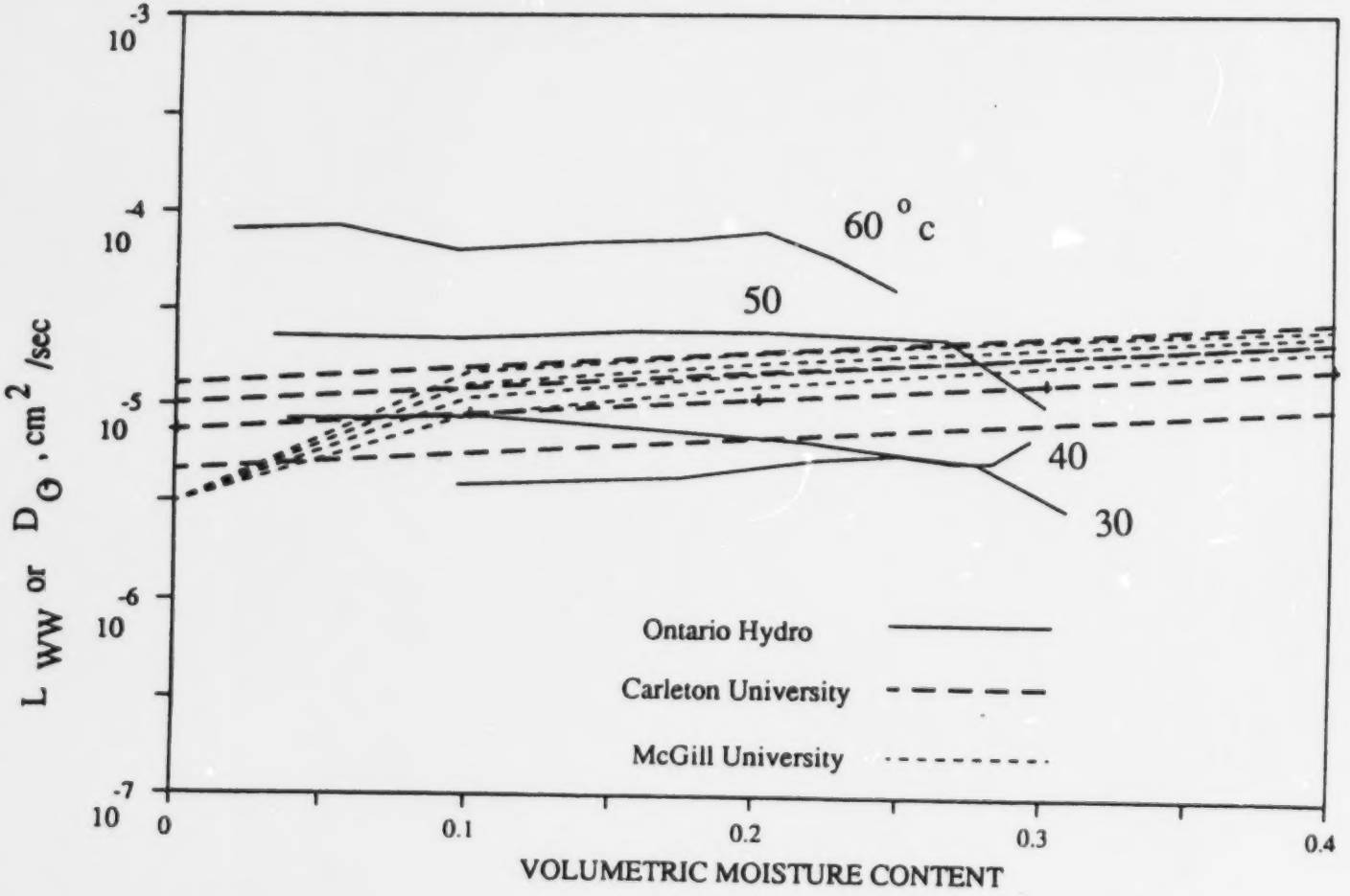


Figure 2 The D_θ or L_{WW} values.

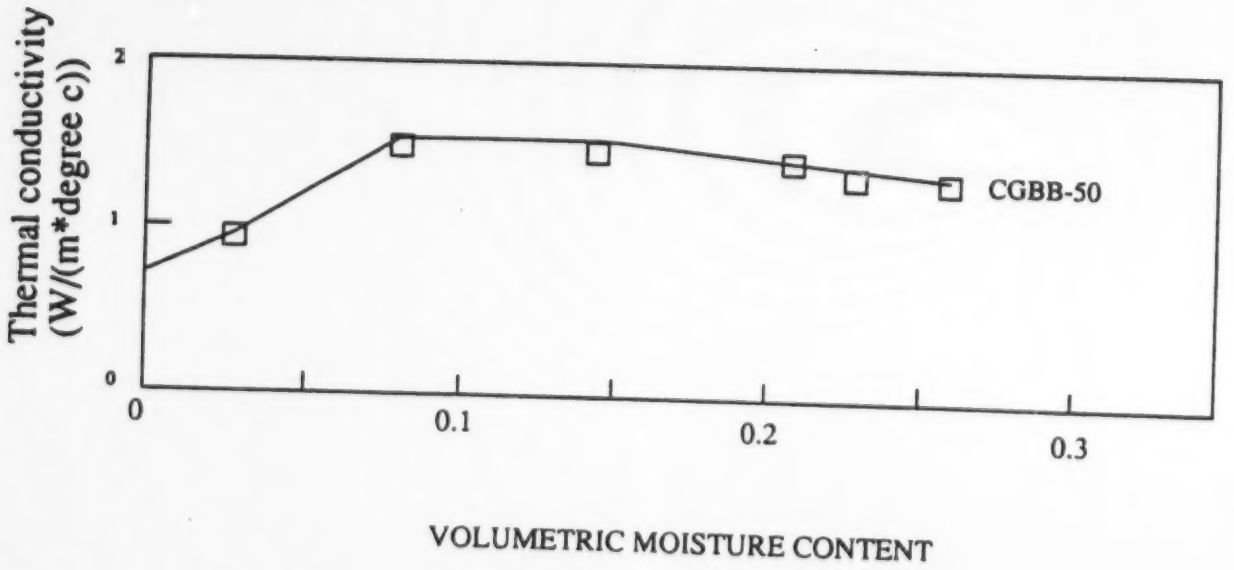


Figure 3 Thermal conductivity of the reference buffer mix.

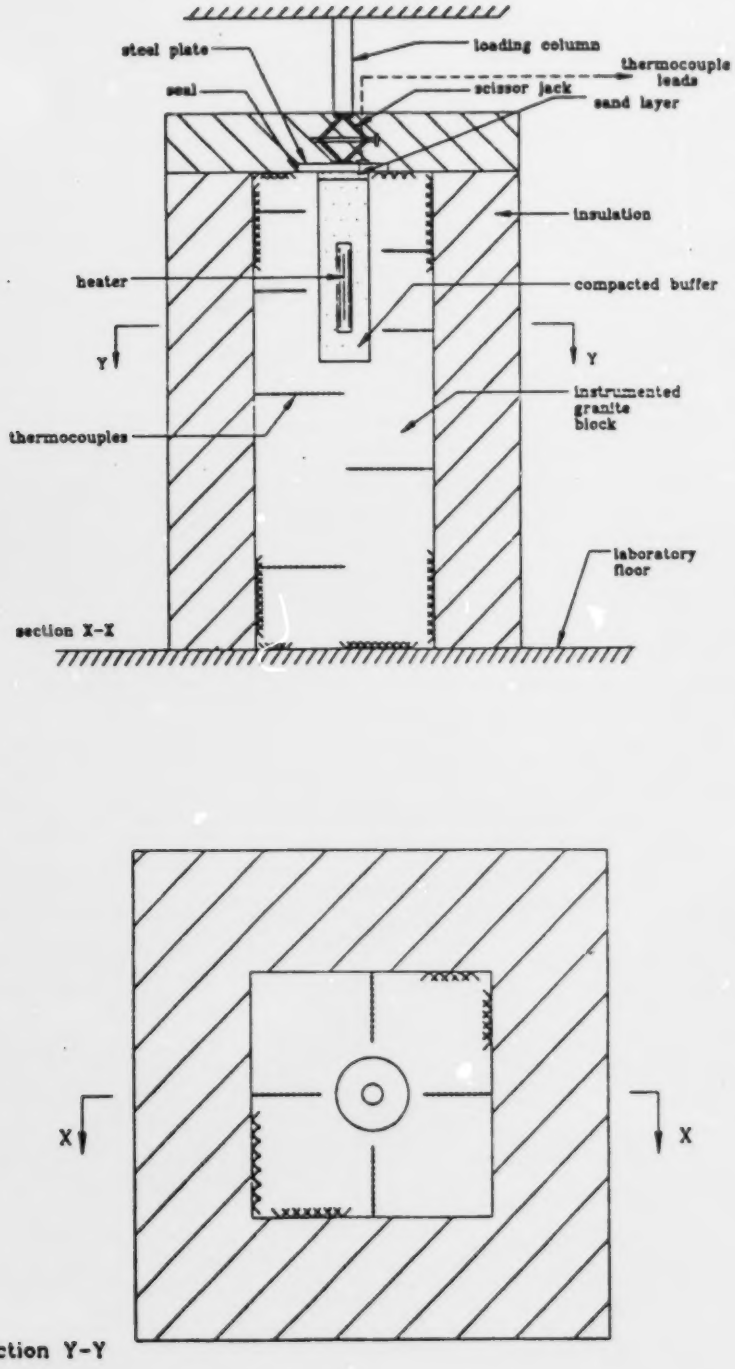
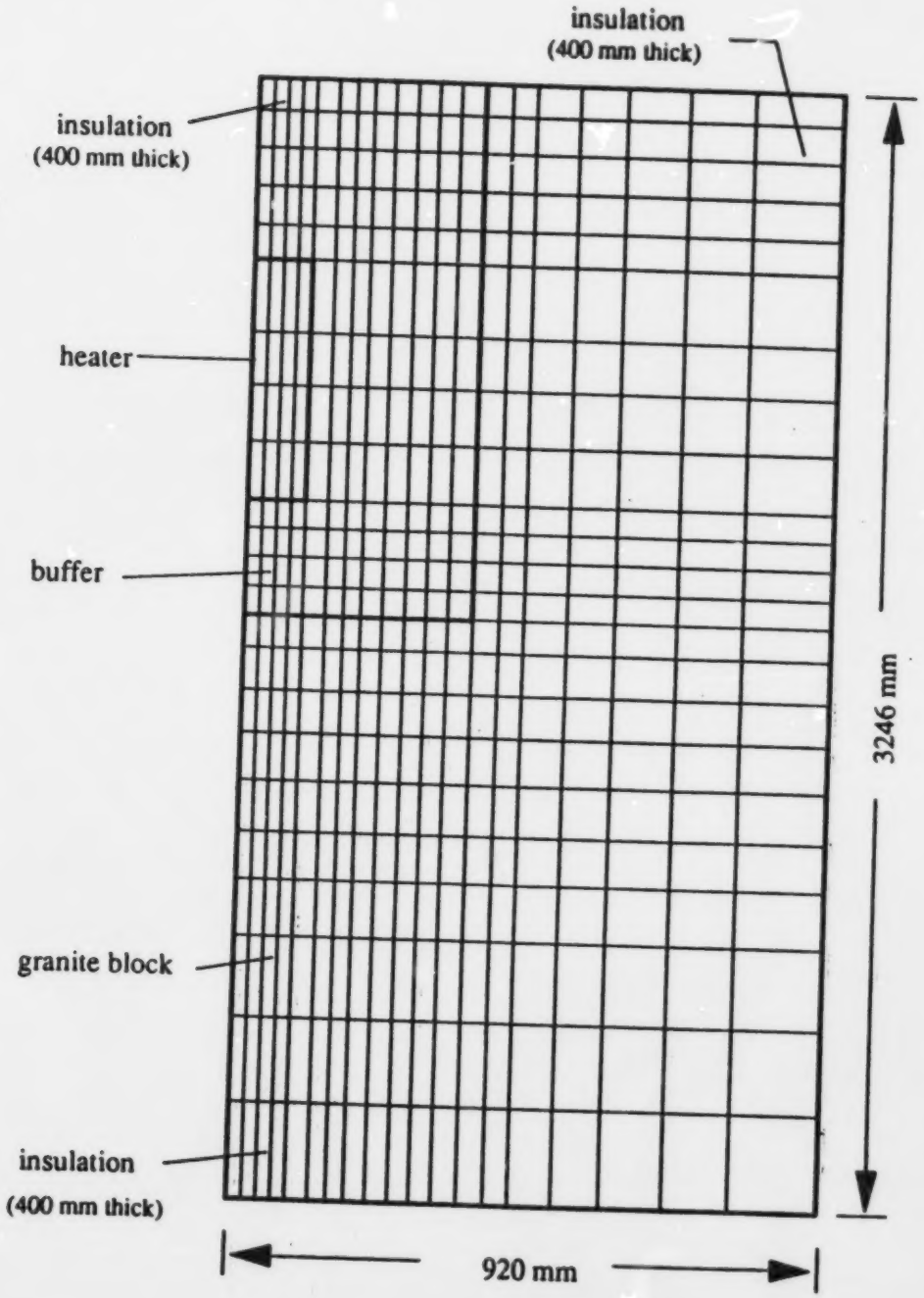


Figure 4 Layout of the granite block experiment.



Not to Scale

Figure 5 The integrated finite difference mesh.

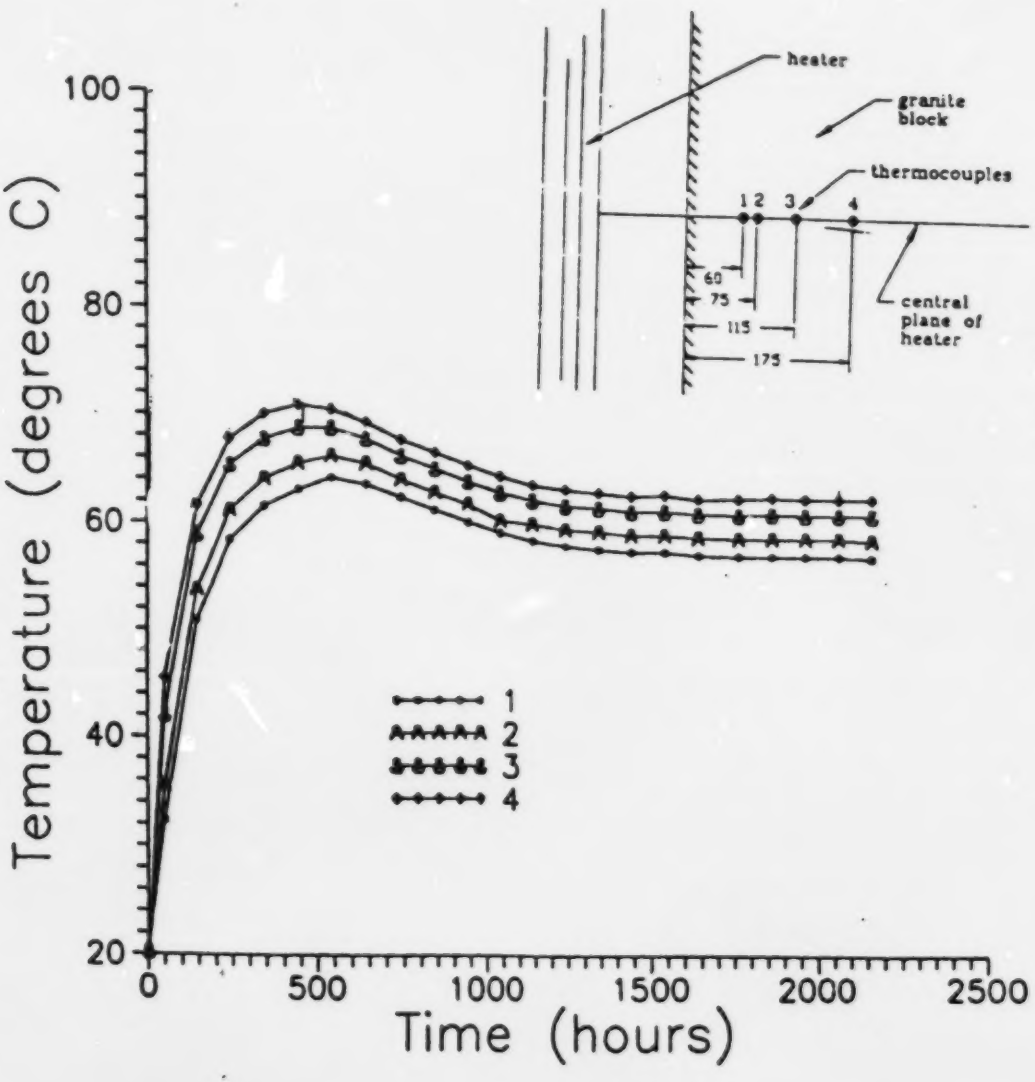


Figure 6 Measured temperature vs. time curves.

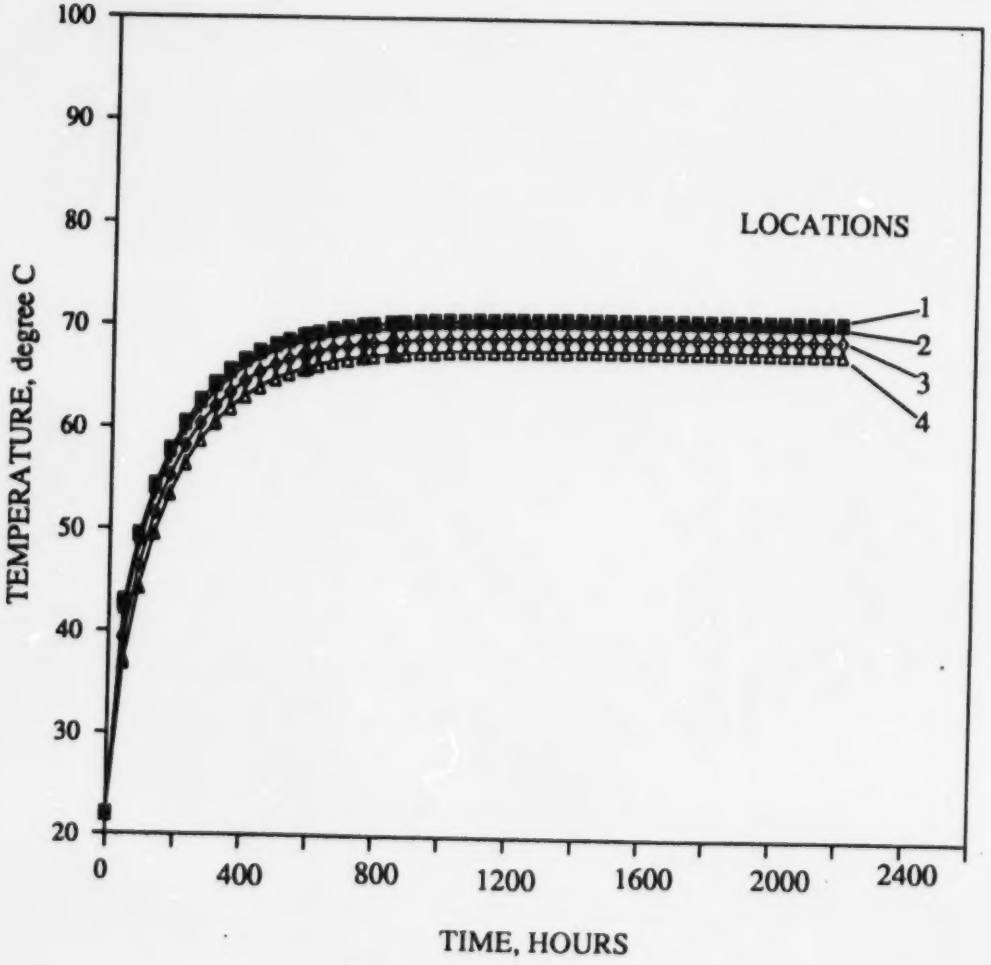


Figure 7 Predicted temperature vs. time curves - Carleton's data.

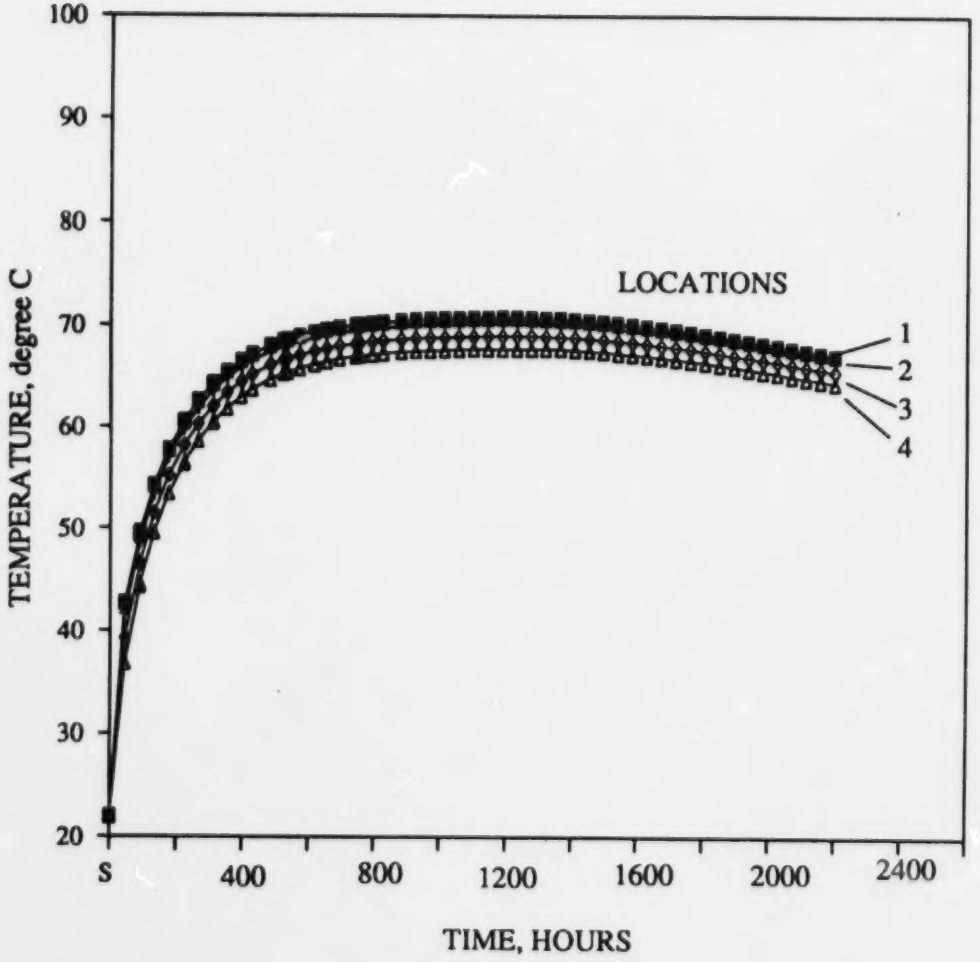


Figure 8 Predicted temperature vs. time curves - McGill's data.

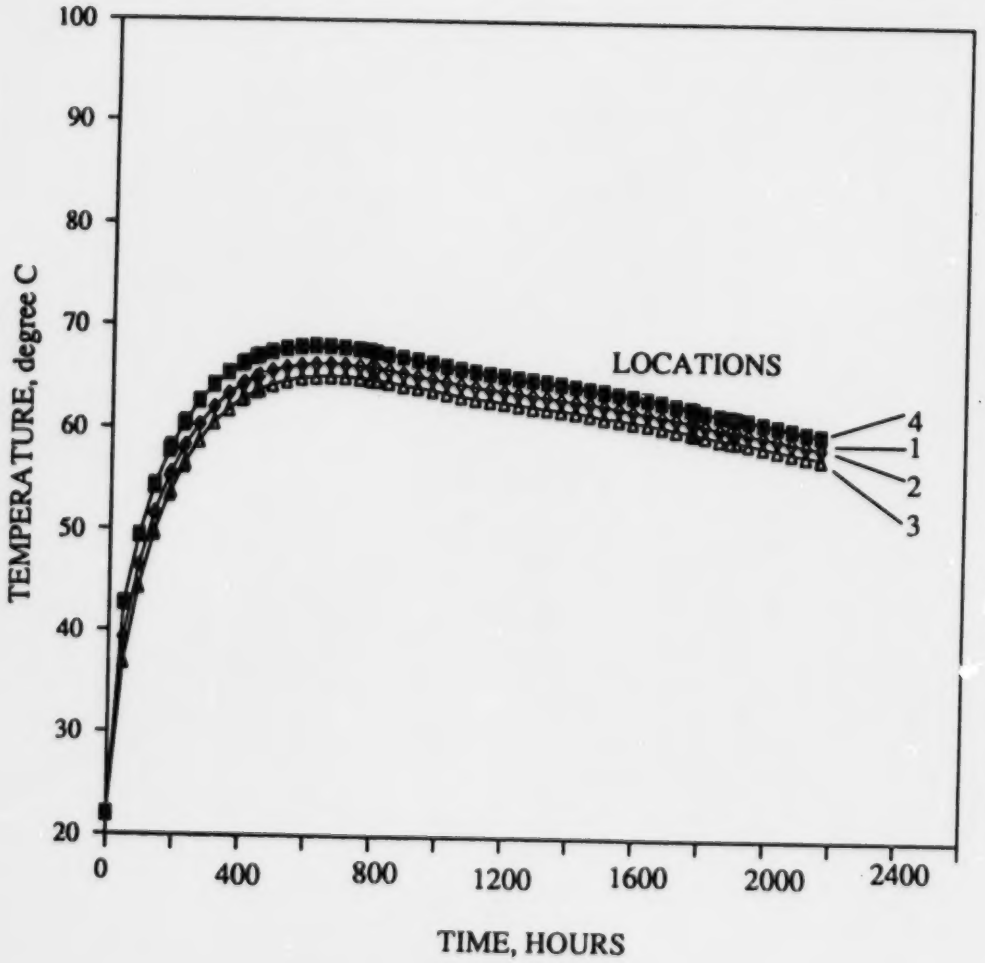


Figure 9 Predicted temperature vs. time curves - Ontario Hydro's data.

Figure 10 The predicted normalized volumetric moisture content profile - Carleton's data.

Figure 11 The predicted normalized volumetric moisture content profile - McGill's data.

Figure 12 The predicted normalized volumetric moisture content profile - Ontario Hydro's data.

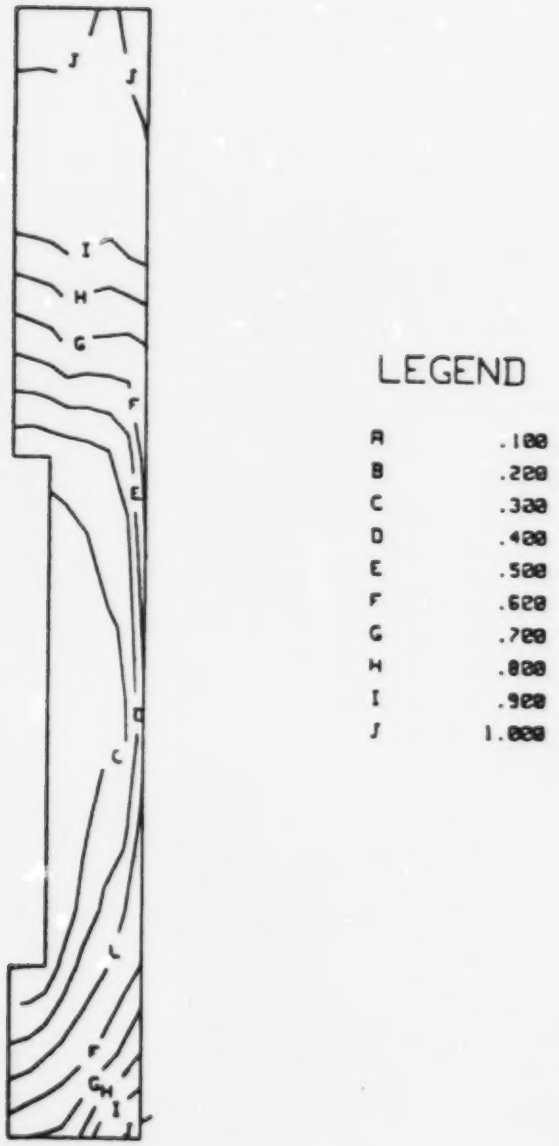


Figure 13 The measured normalized volumetric moisture content profile.

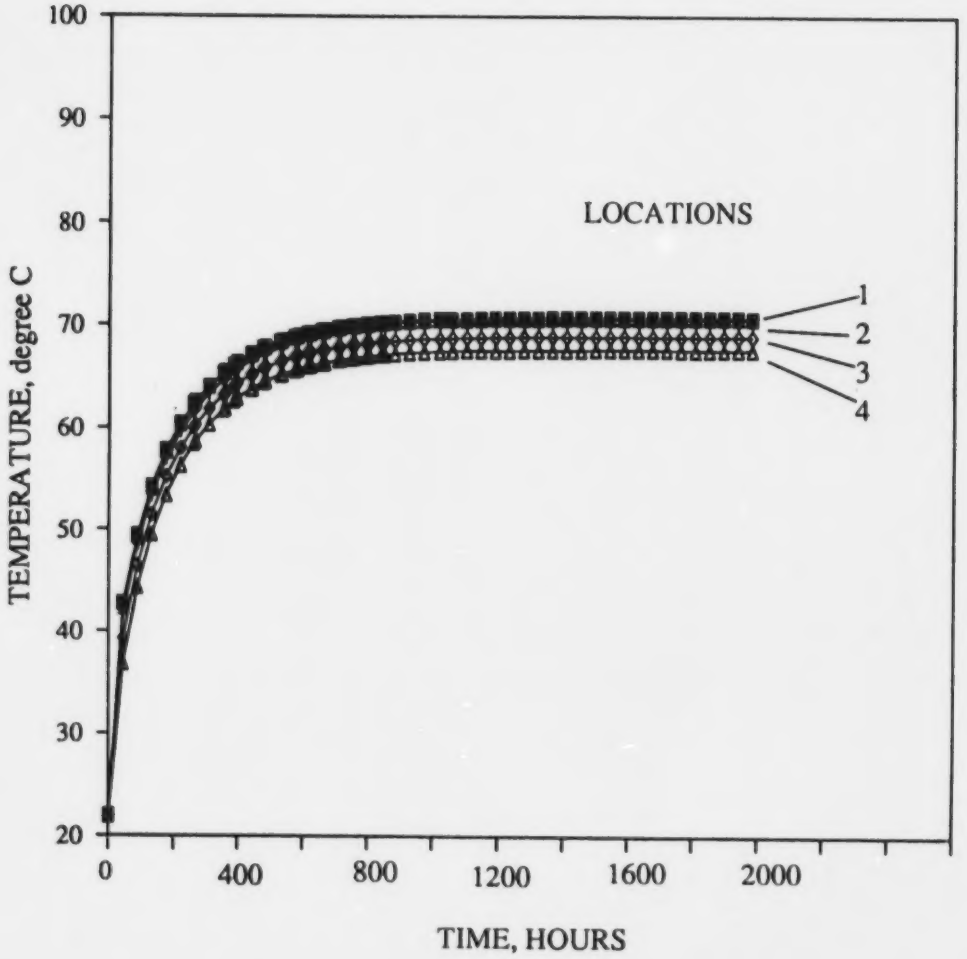


Figure 14 Predicted temperature vs. time curves - impermeable hydraulic boundary condition at buffer/rock interface.

Figure 15 The predicted normalized volumetric moisture content profile - impermeable hydraulic boundary.

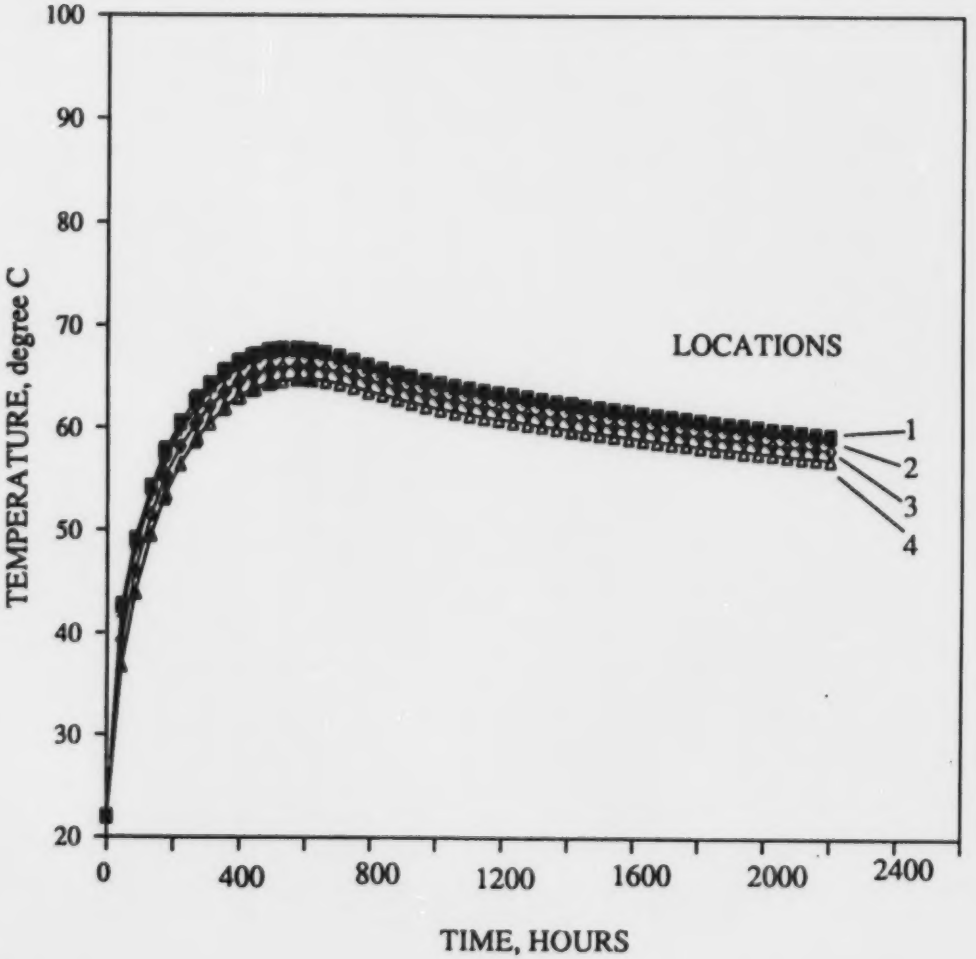


Figure 16 Predicted temperature vs. time curves - with temperature dependent material properties.

Figure 17 The predicted normalized volumetric content profile - with temperature dependent material properties.